Dynamical analysis of the buildup process near resonance

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The time evolution of the buildup process inside a double-barrier system for off-resonance incidence energies is studied by considering the analytic solution of the time dependent Schrödinger equation with cutoff plane wave initial conditions. We show that the buildup process exhibits invariances under arbitrary changes on the system parameters, which can be successfully described by a simple and easy-to-use one-level formula. We find that the buildup of the off-resonant probability density is characterized by an oscillatory pattern modulated by the resonant case which governs the duration of the transient regime. This is evidence that off-resonant and resonant tunneling are two correlated processes, whose transient regime is characterized by the same transient time constant of two lifetimes.

The buildup process of electrons inside the quantum well of a double barrier (DB) resonant structure has been one of the most important problems under investigation since it governs the ultimate speed of high frequency tunneling devices[1,2]. Although the first theoretical efforts to estimate the relevant time scales for this mechanism were based on stationary approaches[2,3], it has been widely recognized that this process is of a dynamical nature[3,4]; hence, the solution of the time-dependent Schrödinger equation provides the most reliable way to tackle this fundamental problem.

In this letter we provide a full quantum dynamical study of the buildup process at resonance and off-resonance incidence energies, based on an exact analytical solution. We show that within the complexity of the process, underlying invariances can be found in the time evolution of the probability density. Important conclusions on the relevant time scale that characterizes both the resonant and off-resonant buildup are brought out from such invariances.

Our analysis deals with the analytic solution of the time-dependent Schrödinger equation for a finite range potential $V(x)$ that vanishes outside the region $0 \leq x \leq L$, with a cutoff plane initial condition,

$$\Psi(x,k;t=0) = \begin{cases} e^{ikx} - e^{-ikx}, & -\infty < x \leq 0, \\ 0, & x > 0, \end{cases} \quad (1)$$

which refers to a perfect reflecting shutter[5]. The solution for the internal region[6] reads,

$$\Psi(x,k;t) = \phi(x,k)M(0,k;t) - \phi^*(x,k)M(0,-k;t)$$

$$-i \sum_{n=-\infty}^{\infty} \phi_n M(0,k_n;t), \quad (2)$$

where $\phi(x)$ stands for the stationary solution, and $\phi_n = 2ku_n(0)u_n(x)/(k^2 - k_n^2)$ is given in terms of the resonant states, $\{u_n(x)\}$, and the $S-$matrix poles, $\{k_n\}$, of the system. The index n runs over the complex poles k_n, distributed in the third and fourth quadrants in the complex k-plane. In the above equation the Moshinsky functions $M(0,q;t)$ are defined in terms of the complex error function $w(z)$, as $M(0,q;t) \equiv M(y_q) = w(iy_q)/2$, where the argument is given by $y_q = -exp(-i\pi/4)(m/2\hbar)^{1/2}\left[(\hbar q/m)t^{1/2}\right]$, and q stands either for $\pm k$ or $k_{\pm n}$.

The formal solution for the internal region, Eq. (2), allows us to study both the spatial behavior and the time evolution of the probability density for any incidence energy $E = \hbar^2 k^2/2m$. The main ingredients of Eq. (2) are the stationary wavefunction $\phi(x,k)$, the resonance parameters $\{E_n = \varepsilon_n - i\Gamma_n/2 = \hbar^2 k_n^2/2m\}$ and the corresponding resonant eigenfunctions $\{u_n(x)\}$. The latter can be obtained by a straightforward calculation using the transfer matrix method adapted to the complex eigenvalue problem[7]. For systems with isolated (non-overlapping) resonances, the single-resonance term approximation to Eq. (2) gives an excellent description, except for very short times ($t \ll \hbar/\Gamma_n$) in which one has to consider contributions from additional resonance terms. In all the numerical examples presented here the single term approximation applies.

As a first example, let us consider the DB struc-

ture (system A) with parameters: barrier heights $V_1 = V_2 = 0.23 \ eV$, barrier widths $b_1 = b_2 = 5.0 \ nm$, well width $\omega_0 = 5.0 \ nm$, and effective mass for the electron $m = 0.067 m_e$. The resonance parameters for the first resonant state are: energy position, $\varepsilon_1 = 80.11 \ meV$, and resonance width, $\Gamma_1 = 1.03 \ meV$. In Fig. 1 (a) we plot $|\Psi|^2$, calculated from Eq. (2), as a function of the position x along the internal region, for specific times $\{t_i\}$ whose increasing values are given in the figure. Here, the incidence energy is chosen below resonance, at $E = 75.0 \ meV$. Note that the off-resonant buildup occurs in such a way that $|\Psi|^2$ is found sometimes above or below the asymptotic value $|\phi|^2$. This behavior is dramatically different from the monotonic growth that characterizes the special case of incidence at resonance, see Fig. 4 of Ref. 8. In order to show the time dependence of the probability density for a fixed position x_0, we plot in part (b) $|\Psi(x_0, k; t)|^2$ versus t for different deviations from resonance $\Delta E = |E - \varepsilon_1|$. Note that $|\Psi|^2$ fluctuates around its asymptotic value $|\phi|^2$, and exhibits an oscillatory behavior not present in the resonant case, as shown in Fig. 1 (b).

Up to here, we have illustrated the behavior of the off-resonance buildup only for a particular potential profile. It is clear that any changes in either the incident energy or the potential profile parameters will affect the solution $\Psi(x, k; t)$ since the relevant input to Eq. (2), namely, $\phi(x, k)$, $u_n(x)$ and E_n, strongly depends on the potential parameters. For instance, let us consider two additional DB systems with potential profiles quite different from system A; the first corresponds to the symmetrical structure (system B) with parameters: barrier heights $V_1 = V_2 = 0.5 \ eV$, barrier widths $b_1 = b_2 = 3.0 \ nm$ and well width $\omega_0 = 10.0 \ nm$; the second corresponds to an asymmetrical structure (system C), whose parameters are: $V_1 = 0.45 \ eV$, $V_2 = 0.35 \ eV$, $b_1 = 3.0 \ nm$, $b_2 = 10.0 \ nm$ and $\omega_0 = 8.0 \ nm$. The resonance parameters for the first eigenstate are: $\varepsilon_1 = 37.80 \ meV$, $\Gamma_1 = 0.12 \ meV$ (system B); and $\varepsilon_1 = 51.29 \ meV$, $\Gamma_1 = 0.17 \ meV$ (system C). The value of the transmission peak $T(\varepsilon_1)$ is unity for A and B; for system C, $T(\varepsilon_1) < 1$, since it is asymmetric. We choose here the incidence energies $E = \varepsilon_1 - \Delta E$ such that the ratio $\gamma = T(E)/T(\varepsilon_1)$ is the same for A, B, and C. For example, if we choose E such that $T(E)$ is 1.0 % of $T(\varepsilon_1)$, from numerical inspection from a T versus E plot (not shown here), the incidence energies for A, B, and C, must be 74.97, 37.20 and 50.44 (meV), respectively. The results of the comparison of the time evolution of $|\Psi|^2$ for this selection ($\gamma = .01$), are shown in Fig. 2 (a). The three curves are strongly different, as expected. Thus, the complete characterization of the buildup process for a broad range of potential geometries seems to be a too involved task; however, one of the purposes of this work is to show that despite this complex situation, the probability density has striking invariances under changes in the potential profiles. To illustrate the above let us consider a more suitable representation for the probability density *i. e.* $|\Psi/\phi|^2$ as a function of τ,

which is the time normalized to lifetime units. We find a striking result: all curves coincide exactly for the three different systems, see Fig. 2 (b). This result suggests the existence of an underlying invariance in the process.

In order to show the existence of such invariance, we derive a one-level formula for the normalized probability density starting from the formal solution (2). We proceed along the same lines discussed in our recent work[9], but considering incidence energies different from resonance ($E \neq \varepsilon_n$). Following such a procedure we obtain,

$$|\Psi(\tau)/\phi|^2 = 1 + e^{-\tau} - 2e^{-\tau/2} \cos[\omega_n \tau], \qquad (3)$$

where $\omega_n = (\varepsilon_n - E)/\Gamma_n$ is a dimensionless frequency. The reliability of this one-level formula is shown in a plot of Eq. (3) included in Fig. 2 (b), and we see an excellent agreement. Furthermore, note that Eq. (3) depends in general on the system parameters through the frequency ω_n; however, it can be shown straightforwardly that the condition previously imposed on the ratio $T(E)/T(\varepsilon_n)$ guarantees the independence of Eq. (3) on the potential profile. Consider the Breit-Wigner expression for the transmission coefficient[7],

$$T(E) = \frac{\Gamma_n^0 \Gamma_n^L}{(E - \varepsilon_n)^2 + \Gamma_n^2/4}, \qquad (4)$$

where Γ_n^0 and Γ_n^L are the partial decay widths of the system which satisfy $\Gamma_n = \Gamma_n^0 + \Gamma_n^L$. This formula of $T(E)$ is valid for isolated non-overlapping resonances, that is $\Gamma_n \ll |\varepsilon_n - \varepsilon_{n\pm1}|$, which is the case of a broad range of typical DB structures. From Eq. (4) we can easily calculate the ratio $\gamma = T(E)/T(\varepsilon_1)$ and obtain an expression for the frequency $\omega_1 = (\gamma^{-1} - 1)^{1/2}/2$. As a consequence, Eq. (3) is no longer dependent on the system parameters since it only depends on γ. Note that the frequency ω_1 also measures the deviations of the incidence energy E from the resonance ε_1 in multiple numbers of Γ_1, *i.e.* $\Delta E = \omega_1 \Gamma_1$. In other words, different systems share the same curve of the probability density provided that deviations from resonance are the same in units of the corresponding resonance width Γ_1. Note also that Eq. (3) is independent of the choice $\pm\omega_n$, which implies that deviations above and below resonance give the same result. Since in our example $\gamma = 0.01$, we have that $\omega_1 \approx 5.0$; this can also be verified by computing the values of $\omega_1 = |\Delta E|/\Gamma_1$ from the incidence energies used in Fig. 2.

Note another interesting regularity of $|\Psi(\tau)/\phi|^2$; the damped oscillatory behavior in Eq. (3) is modulated by the lower envelope

$$|\Psi(\tau)/\phi|^2 = \left(1 - e^{-\tau/\tau_0}\right)^2, \qquad (5)$$

which is exactly the capacitor-like buildup law obtained for the special case of incidence at resonance[9], where the transient time constant τ_0 of the process is exactly two lifetimes, $\tau_0 = 2$. A plot of Eq. (5) is included in Fig.

2 (b). This result is relevant from a physical point of view, since it is a manifestation of the subtle interplay between the incident off-resonant carriers and the quasibound state of the system: resonant and off-resonant buildup, although different processes, are not uncorrelated at all, the latter is governed by the former in the way exhibited in Fig. 2(b). As a consequence, the transient regime for both situations is characterized by the same transient time constant τ_0. The above mentioned quantity is relevant for the design and optimization of resonant tunneling diodes; in this respect, a detailed discussion can be found in a recent work by Luryi and Zaslavsky[10], in which the distinction between capacitive and quantum contributions to an effective time constant is analyzed.

In conclusion, the dynamics of the buildup mechanism at off-resonance incidence energies has been explored in typical DB resonant structures. We have shown that, despite the complexity that characterizes the dynamical process, the time evolution of the probability density exhibits invariances under arbitrary changes on the system parameters. From such invariances we conclude that the transient regime in both resonant and off-resonant processes is characterized by the same transient time constant of two lifetimes. Our results are valid for any DB system with isolated resonances and incident plane wave initial condition.

FIG. 1. (a) The birth of $|\Psi|^2$ inside the structure as a function of the position x, for increasing values of time: $t_1 = 0.04$ ps, $t_2 = 0.4$ ps $t_3 = 0.8$ ps, and $t_4 = 1.2$ ps (solid lines). The stationary solution $|\phi|^2$ (dashed line) is also included for comparison. (b) The time evolution of $|\Psi|^2$ at the fixed position at the center of the well, for different values of $\Delta E = \Delta E_k$, where: $\Delta E_1 = 0.6, \Delta E_2 = 1.1$, and $\Delta E_3 = 1.6$ (meV).

FIG. 2. (a) The time evolution of $|\Psi|^2$ in the center of the well at off-resonance incidence energy using Eq. (2) for systems A, B, and C. (b) Also from Eq. (2), shows the time evolution of $|\Psi(\tau)/\phi|^2$ as a function of the time τ given now in lifetime units; the curves of A, B and C are indistinguishable among them. The calculation using the one-level formula, Eq. (3), is also included in (b) for comparison and is indistinguishable from A, B, and C. The lower envelope calculated from Eq. (5) is also shown.

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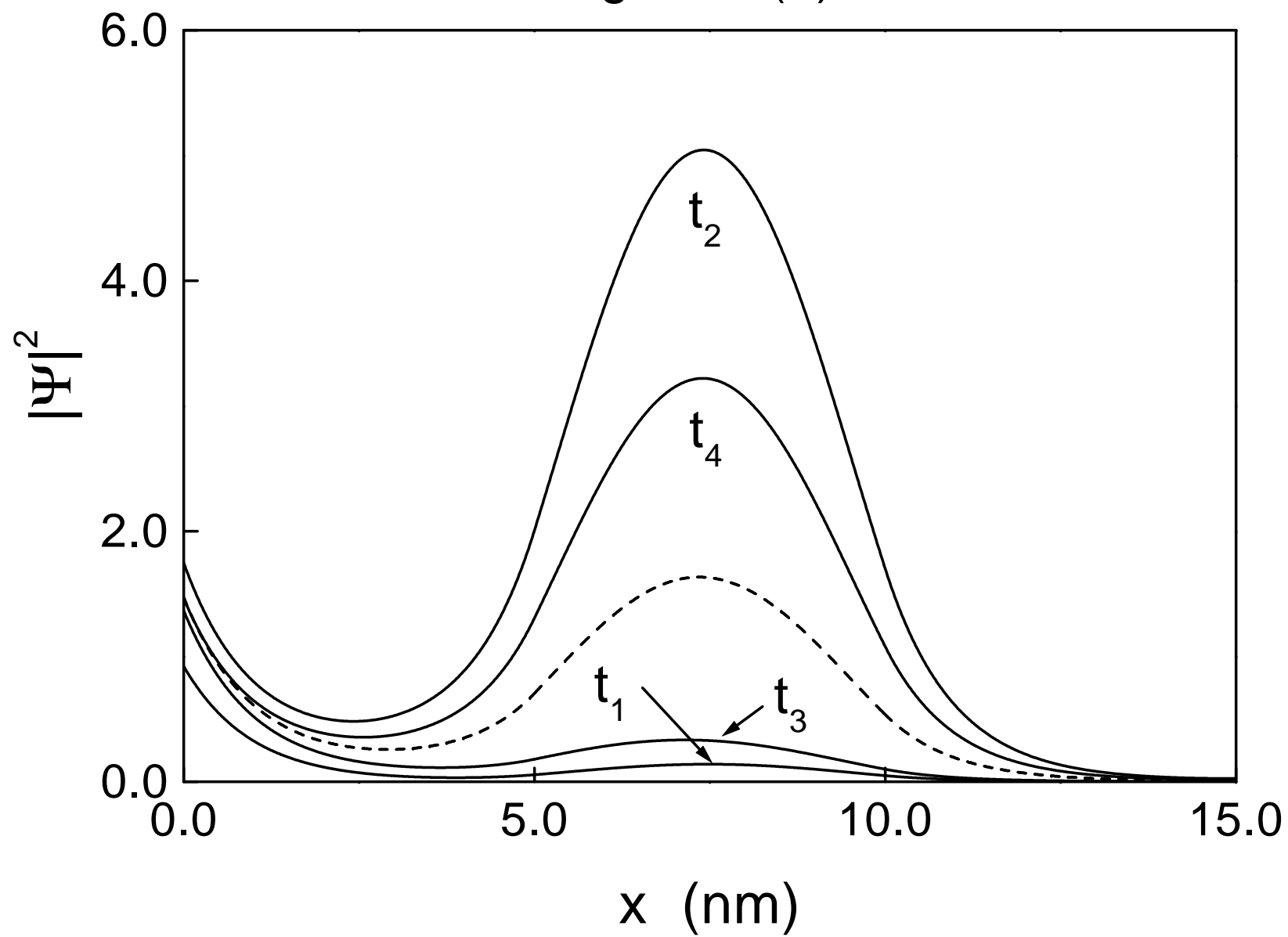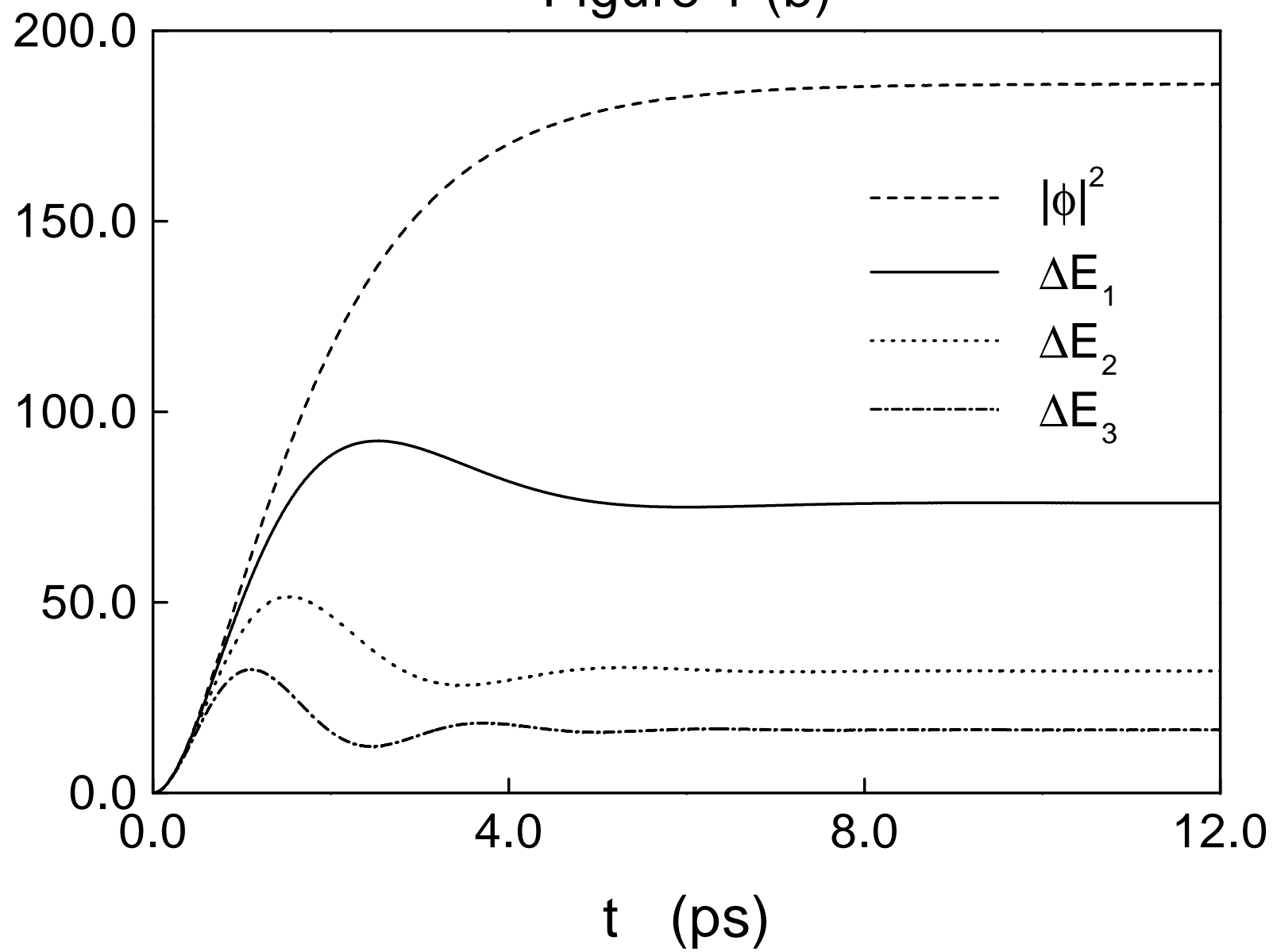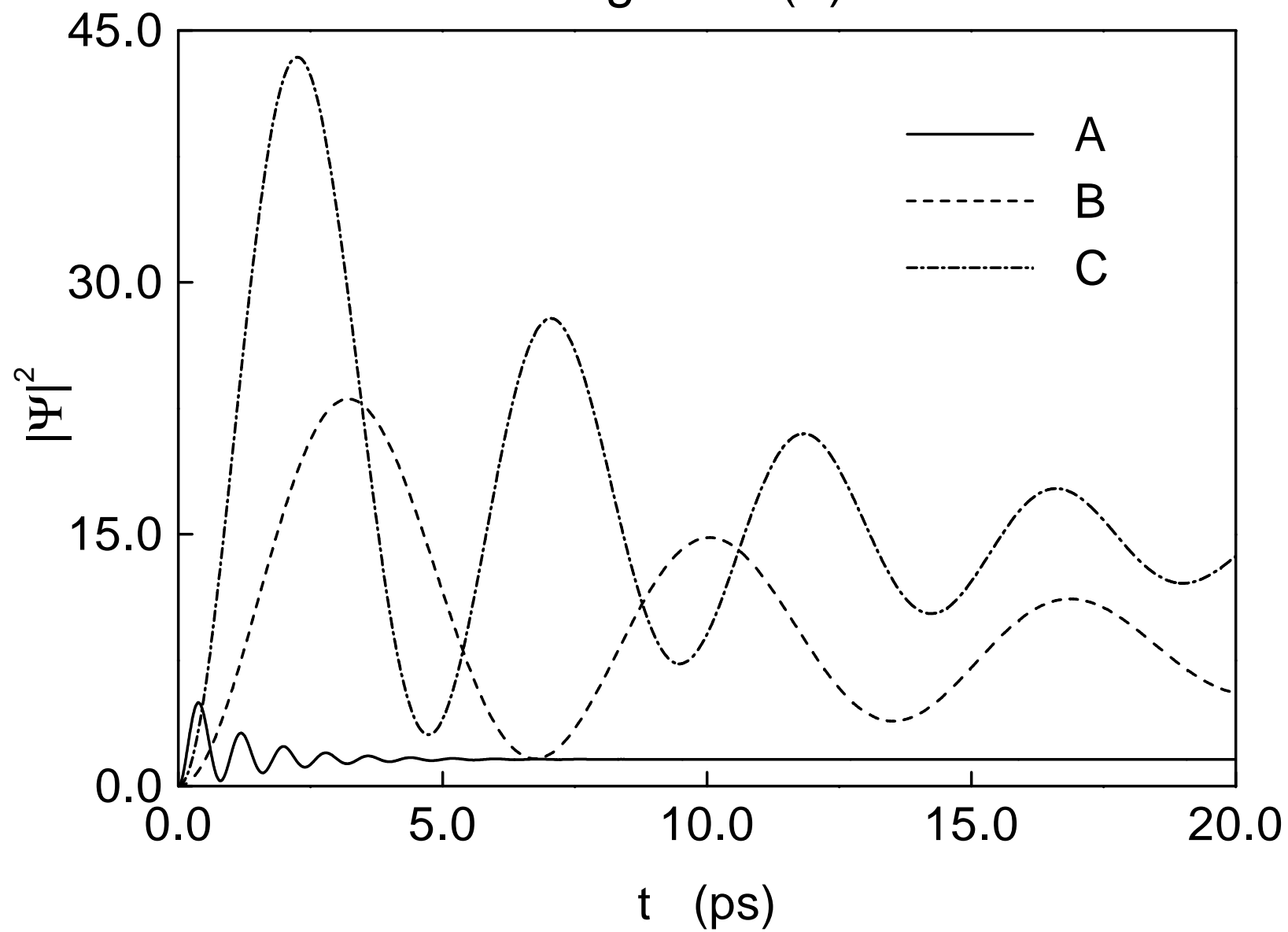
Figure 1 (a)

Figure 1 (b)

Figure 2 (a)

Figure 2 (b)